OBLON, SPIVAK, et al.
SERIAL NO:09/877,182
INV: Beau HANSEN, ET AL.
DOCKET # 204931US-20

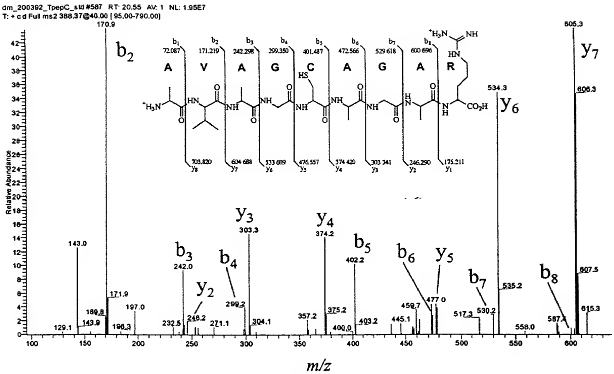


FIG. 1

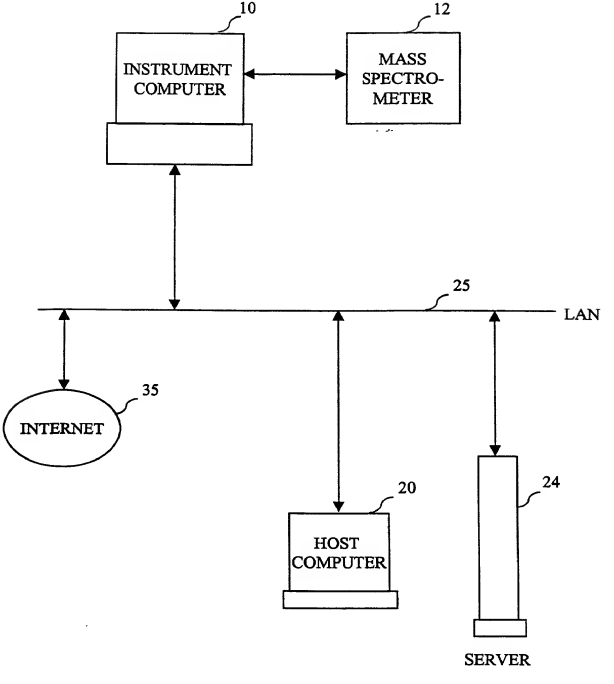

10
INSTRUMENT COMPUTER
12
MASS SPECTRO-METER
25
LAN
35
INTERNET
20
HOST COMPUTER
24
SERVER

FIG. 2

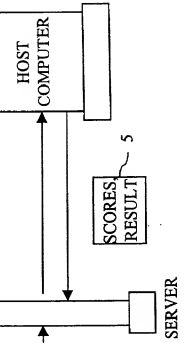

20
HOST COMPUTER
3
RAW DATA FILE
5
SCORES RESULT
24
SERVER
3
RAW DATA FILE
10
INSTRUMENT COMPUTER
1
RAW DATA
12
MASS SPECTRO-METER

FIG. 3

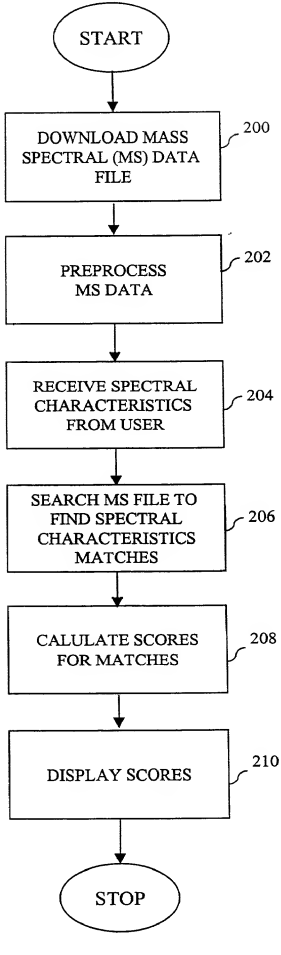

START
DOWNLOAD MASS SPECTRAL (MS) DATA FILE
200
PREPROCESS MS DATA
202
RECEIVE SPECTRAL CHARACTERISTICS FROM USER
204
SEARCH MS FILE TO FIND SPECTRAL CHARACTERISTICS MATCHES
206
CALULATE SCORES FOR MATCHES
208
DISPLAY SCORES
210
STOP

FIG. 4

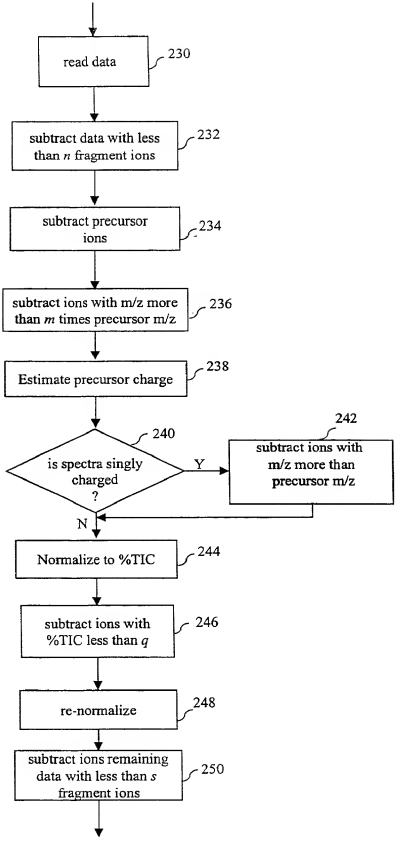

read data
230
subtract data with less than n fragment ions
232
subtract precursor ions
234
subtract ions with m/z more than m times precursor m/z
236
Estimate precursor charge
238
is spectra singly charged ?
240
Y
242
subtract ions with m/z more than precursor m/z
N
Normalize to %TIC
244
subtract ions with %TIC less than q
246
re-normalize
248
subtract ions remaining data with less than s fragment ions
250

FIG. 5

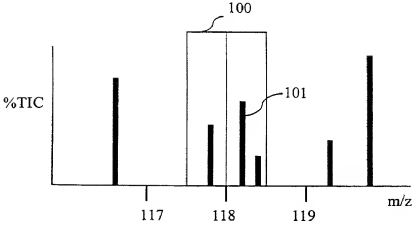


FIG. 6A

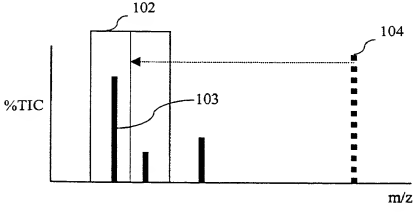


FIG. 6B

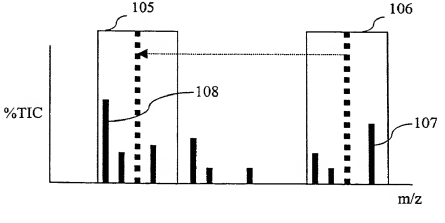


FIG. 6C

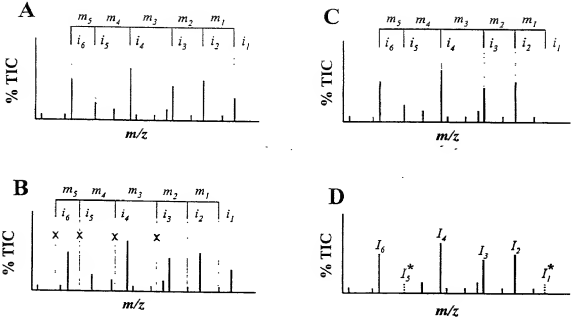
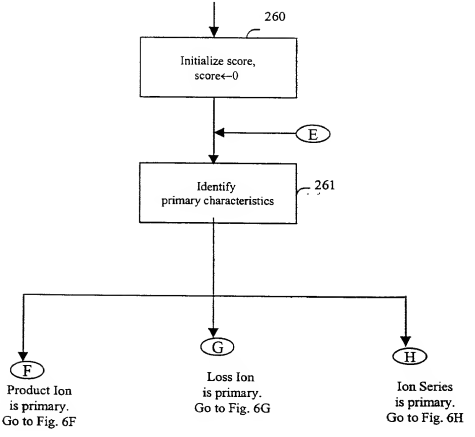


Fig. 6D

FIG. 6E


260
Initialize score,
score←0
E
Identify
primary characteristics
261
F
Product Ion
is primary.
Go to Fig. 6F
G
Loss Ion
is primary.
Go to Fig. 6G
H
Ion Series
is primary.
Go to Fig. 6H

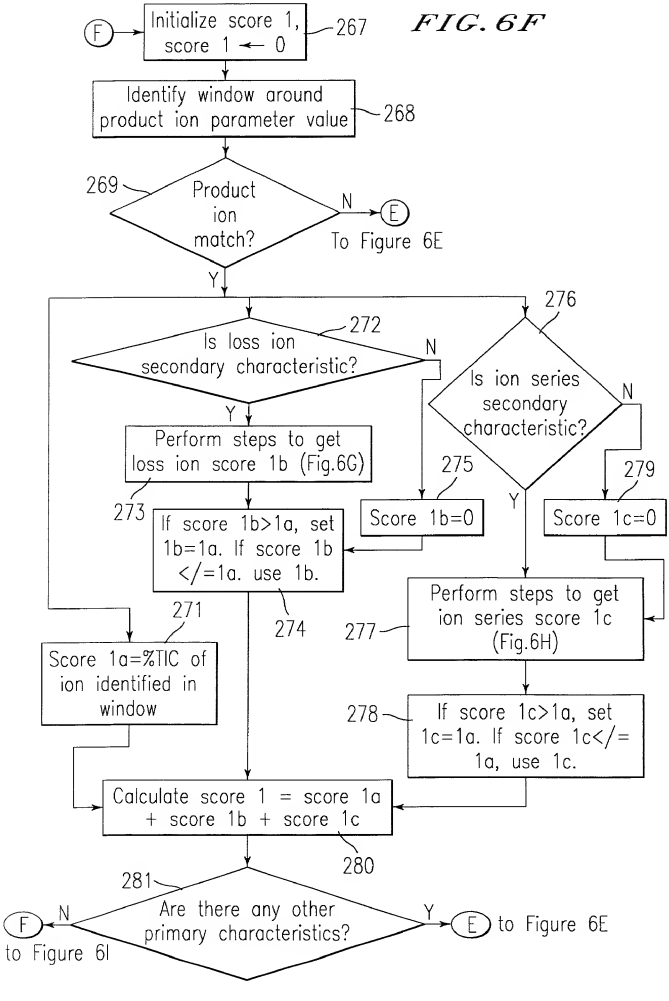
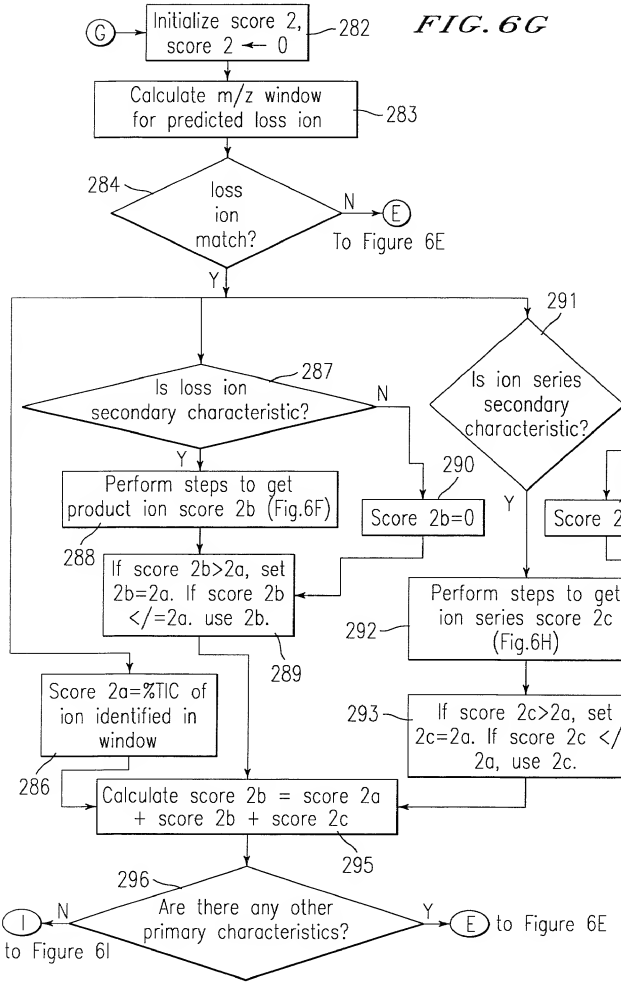


FIG. 6F

FIG. 6G


G
Initialize score 2, score 2 ← 0
282
Calculate m/z window for predicted loss ion
283
284
loss ion match?
N
E
To Figure 6E
Y
291
Is loss ion secondary characteristic?
287
N
Y
Is ion series secondary characteristic?
N
Y
290
294
Perform steps to get product ion score 2b (Fig.6F)
Score 2b=0
Score 2c=0
288
If score 2b>2a, set 2b=2a. If score 2b </=2a. use 2b.
289
Perform steps to get ion series score 2c (Fig.6H)
292
Score 2a=%TIC of ion identified in window
293
If score 2c>2a, set 2c=2a. If score 2c </= 2a, use 2c.
286
Calculate score 2b = score 2a + score 2b + score 2c
295
296
Are there any other primary characteristics?
N
I
to Figure 6I
Y
E
to Figure 6E

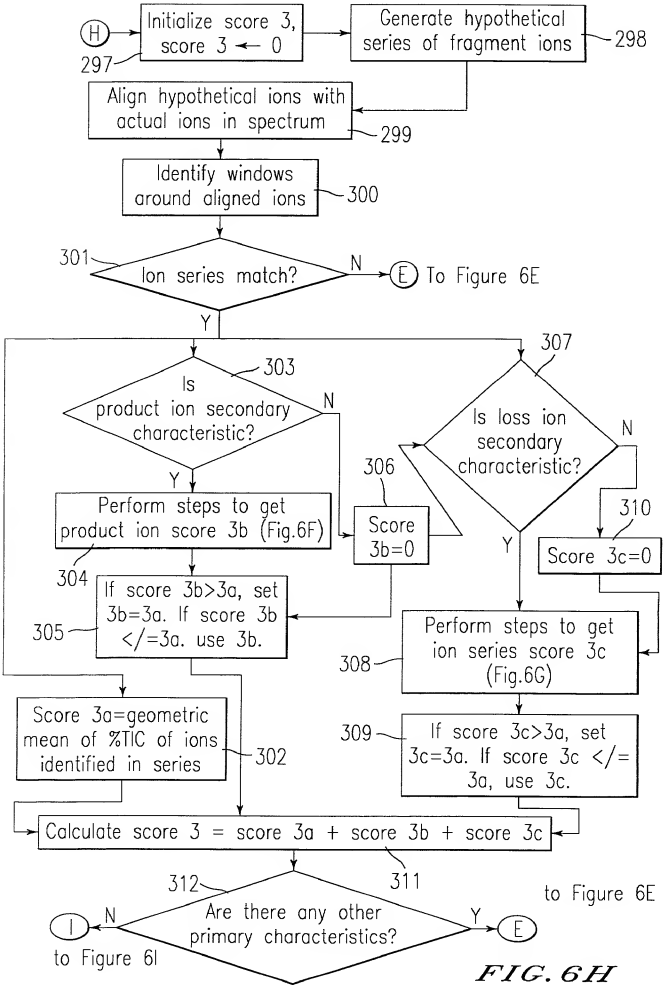

H
Initialize score 3, score 3 ← 0
297
Generate hypothetical series of fragment ions
298
Align hypothetical ions with actual ions in spectrum
299
Identify windows around aligned ions
300
301
Ion series match?
N
E
To Figure 6E
Y
303
Is product ion secondary characteristic?
N
Y
Perform steps to get product ion score 3b (Fig.6F)
304
If score 3b>3a, set 3b=3a. If score 3b </=3a. use 3b.
305
Score 3a=geometric mean of %TIC of ions identified in series
302
306
Score 3b=0
307
Is loss ion secondary characteristic?
N
Y
310
Score 3c=0
Perform steps to get ion series score 3c (Fig.6G)
308
If score 3c>3a, set 3c=3a. If score 3c </= 3a, use 3c.
309
Calculate score 3 = score 3a + score 3b + score 3c
311
312
Are there any other primary characteristics?
N
Y
I
E
to Figure 6I
to Figure 6E

FIG. 6H

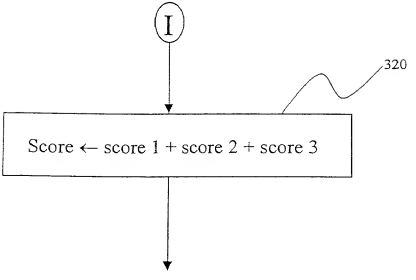


Fig. 6I

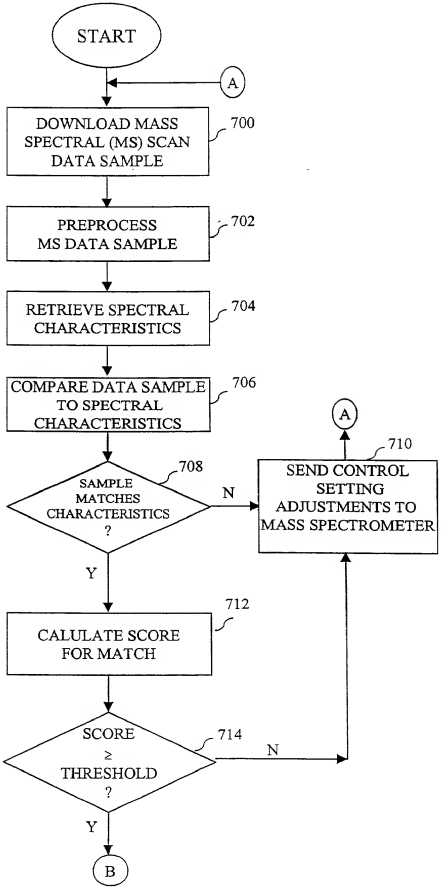

START
A
DOWNLOAD MASS SPECTRAL (MS) SCAN DATA SAMPLE
700
PREPROCESS MS DATA SAMPLE
702
RETRIEVE SPECTRAL CHARACTERISTICS
704
COMPARE DATA SAMPLE TO SPECTRAL CHARACTERISTICS
706
SAMPLE MATCHES CHARACTERISTICS ?
708
N
A
710
SEND CONTROL SETTING ADJUSTMENTS TO MASS SPECTROMETER
Y
CALULATE SCORE FOR MATCH
712
SCORE ≥ THRESHOLD ?
714
N
Y
B

FIG. 7A

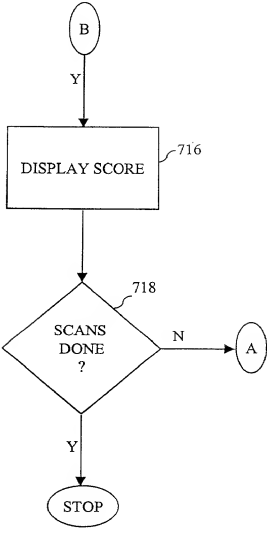


FIG. 7B

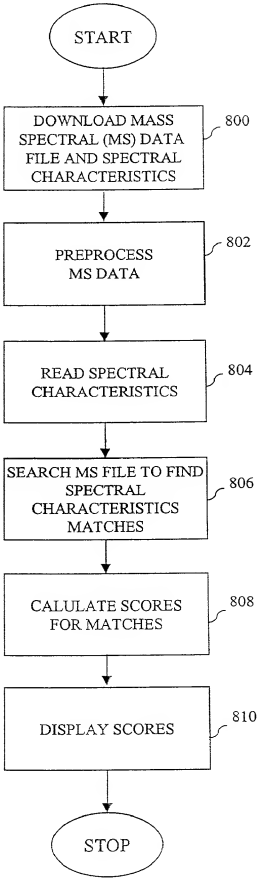

START
DOWNLOAD MASS SPECTRAL (MS) DATA FILE AND SPECTRAL CHARACTERISTICS
800
PREPROCESS MS DATA
802
READ SPECTRAL CHARACTERISTICS
804
SEARCH MS FILE TO FIND SPECTRAL CHARACTERISTICS MATCHES
806
CALULATE SCORES FOR MATCHES
808
DISPLAY SCORES
810
STOP

FIG. 8

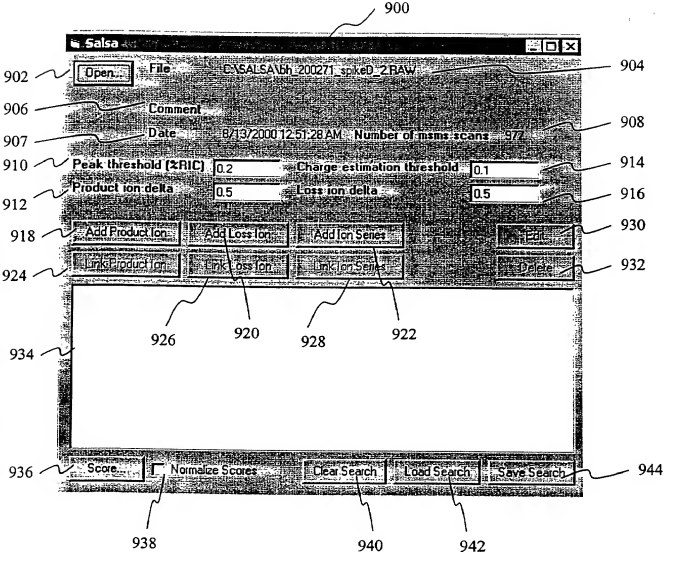

900
Salsa
902
Open...
File
C:\SALSA\5h_200271_spl6D_2.RAW
904
906
Comment
907
Date
8/13/2000 12:51:28 AM
Number of msms scans
972
908
910
Peak threshold (%RIC)
0.2
Charge estimation threshold
0.1
914
912
Product ion delta
0.5
Loss ion delta
0.5
916
918
Add Product Ion
Add Loss Ion
Add Ion Series
Exit
930
924
Link Product Ion
Link Loss Ion
Link Ion Series
Delete
932
926
920
928
922
934
936
Score
Normalize Scores
Clear Search
Load Search
Save Search
944
938
940
942

FIG. 9

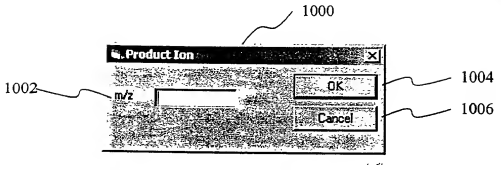

1000
Product Ion
m/z
OK
Cancel
1002
1004
1006

FIG. 10

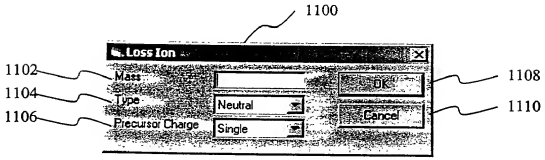

1100
Loss Ion
Mass
Type
Precursor Charge
Neutral
Single
OK
Cancel
1102
1104
1106
1108
1110

FIG. 11

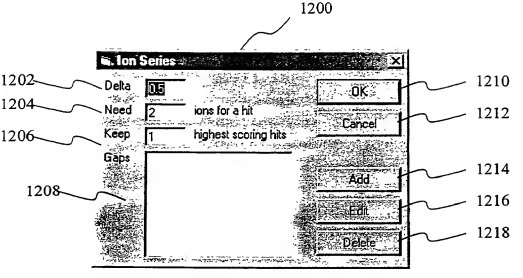

1200
Ion Series
1202
Delta
0.5
1204
Need
2
ions for a hit
1206
Keep
1
highest scoring hits
Gaps
1208
OK
Cancel
Add
Edit
Delete
1210
1212
1214
1216
1218

FIG. 12

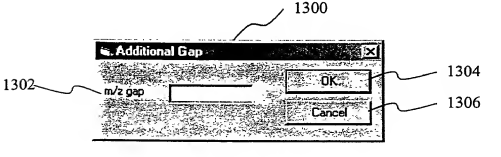

1300
Additional Gap
1302
m/z gap
OK
Cancel
1304
1306

FIG. 13

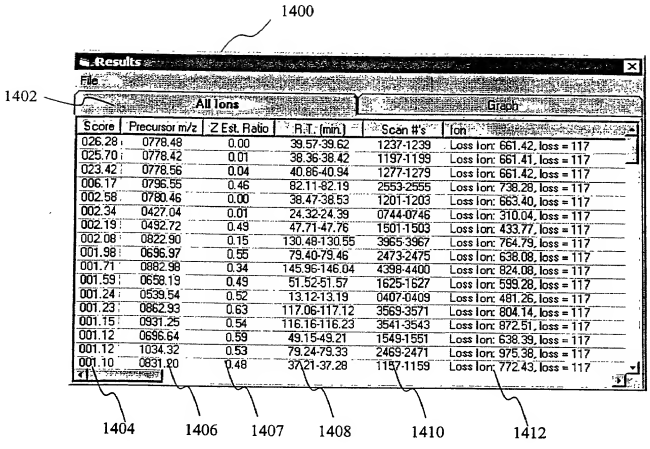
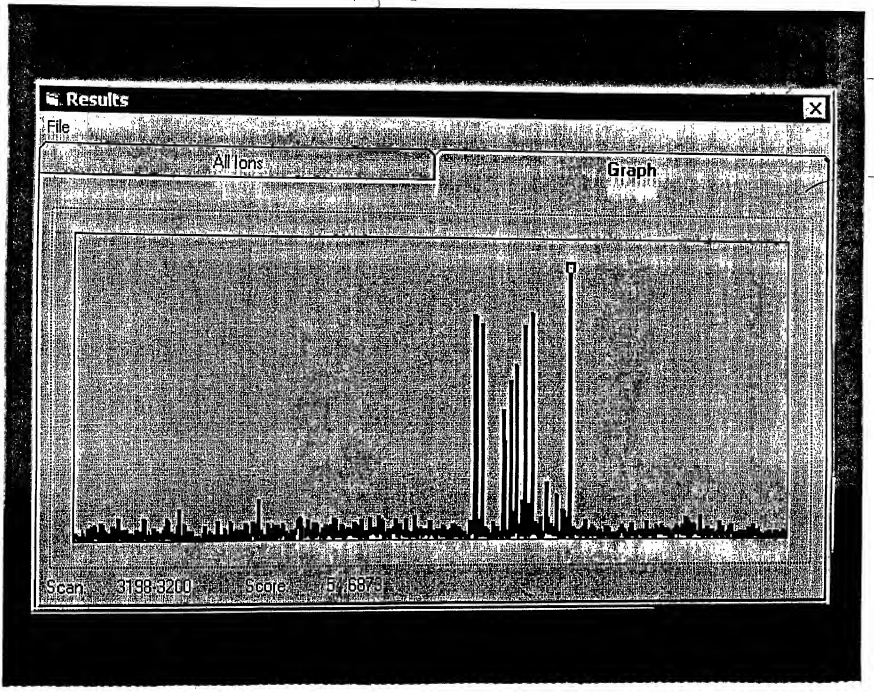

1400
1402
Results
File
All Ions
Graph
Score
Precursor m/z
Z Est. Ratio
R.T. (min.)
Scan #'s
Ion
026.28 0778.48 0.00 39.57-39.62 1237-1239 Loss Ion: 661.42, loss = 117
025.70 0778.42 0.01 38.36-38.42 1197-1199 Loss Ion: 661.41, loss = 117
023.42 0778.56 0.04 40.86-40.94 1277-1279 Loss Ion: 661.42, loss = 117
006.17 0796.55 0.46 82.11-82.19 2553-2555 Loss Ion: 738.28, loss = 117
002.58 0780.46 0.00 38.47-38.53 1201-1203 Loss Ion: 663.40, loss = 117
002.34 0427.04 0.01 24.32-24.39 0744-0746 Loss Ion: 310.04, loss = 117
002.19 0492.72 0.49 47.71-47.76 1501-1503 Loss Ion: 433.77, loss = 117
002.08 0822.90 0.15 130.48-130.55 3965-3967 Loss Ion: 764.79, loss = 117
001.98 0696.97 0.55 79.40-79.46 2473-2475 Loss Ion: 638.08, loss = 117
001.71 0882.98 0.34 145.96-146.04 4398-4400 Loss Ion: 824.08, loss = 117
001.59 0658.19 0.49 51.52-51.57 1625-1627 Loss Ion: 599.28, loss = 117
001.24 0539.54 0.52 13.12-13.19 0407-0409 Loss Ion: 481.26, loss = 117
001.23 0862.93 0.63 117.06-117.12 3569-3571 Loss Ion: 804.14, loss = 117
001.15 0931.25 0.54 116.16-116.23 3541-3543 Loss Ion: 872.51, loss = 117
001.12 0696.64 0.59 49.15-49.21 1549-1551 Loss Ion: 638.39, loss = 117
001.12 1034.32 0.53 79.24-79.33 2469-2471 Loss Ion: 975.38, loss = 117
001.10 0831.20 0.48 37.21-37.28 1157-1159 Loss Ion: 772.43, loss = 117
1404
1406
1407
1408
1410
1412

FIG. 14

Figure 15



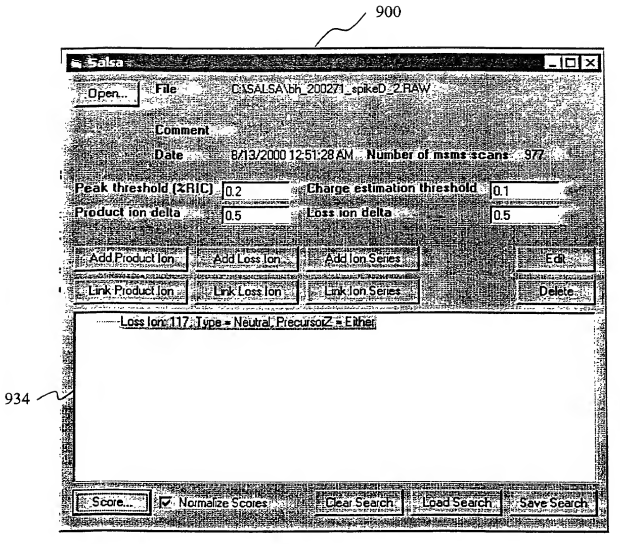

900
Salsa
Open...
File
C:\SALSA\bh_200271_spike0_2.RAW
Comment
Date
8/13/2000 12:51:28 AM
Number of msms scans
977
Peak threshold (%RIC)
0.2
Charge estimation threshold
0.1
Product ion delta
0.5
Loss ion delta
0.5
Add Product Ion
Add Loss Ion
Add Ion Series
Edit
Link Product Ion
Link Loss Ion
Link Ion Series
Delete
Loss Ion: 117, Type = Neutral, PrecursorZ = Either
934
Score...
Normalize Scores
Clear Search
Load Search
Save Search

FIG. 16

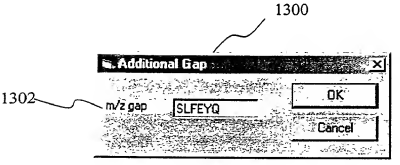

1300
Additional Gap
1302
m/z gap
SLFEYQ
OK
Cancel

FIG. 17

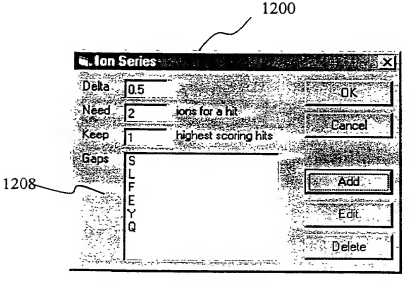

1200
Ion Series
Delta
0.5
OK
Need
2
ions for a hit
Cancel
Keep
1
highest scoring hits
Gaps
1208
S
L
F
E
Y
Q
Add
Edit
Delete

FIG. 18

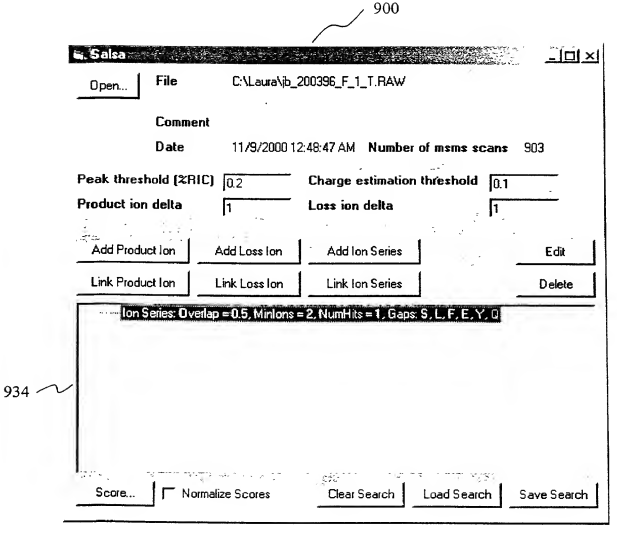

900
Salsa
Open...
File
C:\Laura\jb_200396_F_1_T.RAW
Comment
Date
11/9/2000 12:48:47 AM
Number of msms scans
903
Peak threshold (%RIC)
0.2
Charge estimation threshold
0.1
Product ion delta
1
Loss ion delta
1
Add Product Ion
Add Loss Ion
Add Ion Series
Edit
Link Product Ion
Link Loss Ion
Link Ion Series
Delete
Ion Series: Overlap = 0.5, MinIons = 2, NumHits = 1, Gaps: S, L, F, E, Y, 0
934
Score...
Normalize Scores
Clear Search
Load Search
Save Search

FIG. 19

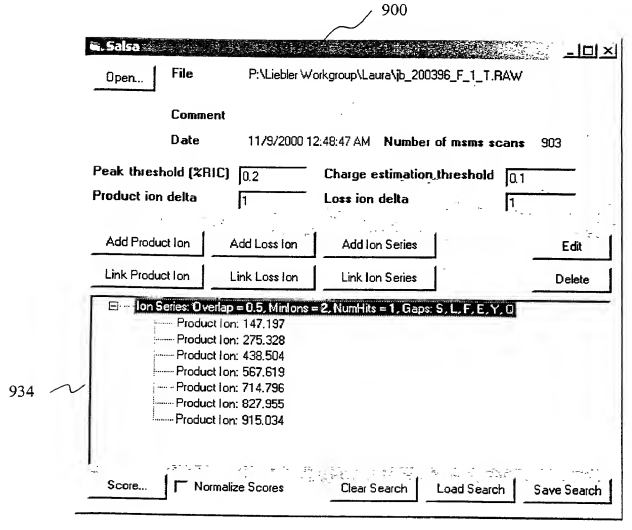

900
Salsa
Open...
File
P:\Liebler Workgroup\Laura\jb_200396_F_1_T.RAW
Comment
Date
11/9/2000 12:48:47 AM
Number of msms scans
903
Peak threshold (%RIC)
0.2
Charge estimation threshold
0.1
Product ion delta
1
Loss ion delta
1
Add Product Ion
Add Loss Ion
Add Ion Series
Edit
Link Product Ion
Link Loss Ion
Link Ion Series
Delete
Ion Series: Overlap = 0.5, MinIons = 2, NumHits = 1, Gaps: S, L, F, E, Y, 0
Product Ion: 147.197
Product Ion: 275.328
Product Ion: 438.504
Product Ion: 567.619
Product Ion: 714.796
Product Ion: 827.955
Product Ion: 915.034
934
Score...
Normalize Scores
Clear Search
Load Search
Save Search

FIG. 20

1400

Results

File

All Ions | Graph

Score	Precursor m/z	Z Est. Ratio	R.T. (min.)	Scan #'s	Ion
012.14	0515.08	0.57	76.82-76.89	2179-2181	Ion Series: 147.01--438.18--567.24
007.20	1028.40	0.02	76.95-77.03	2183-2185	Ion Series: 438.23--567.29--714.21
005.28	0560.65	0.41	71.47-71.54	2027-2029	Ion Series: 210.92--374.07--502.97
005.05	1057.21	0.69	121.76-121.84	3411-3413	Ion Series: 1398.32--1251.37--958.
003.55	1184.04	0.45	131.97-132.04	3687-3689	Ion Series: 1200.67--1328.62--149
003.46	0866.33	0.31	48.29-48.37	1371-1373	Ion Series: 382.23--510.10--673.86
003.44	0750.14	0.65	130.29-130.37	3639-3641	Ion Series: 315.33--606.91--736.05
003.38	0546.80	0.50	67.65-67.72	1919-1921	Ion Series: 359.22--506.33--619.16
003.33	1247.68	0.49	131.27-131.35	3667-3669	Ion Series: 1200.67--1328.67--149
003.20	0993.64	0.46	120.06-120.14	3367-3369	Ion Series: 814.40--1090.61--1203.
003.12	0423.89	0.61	61.85-61.92	1755-1757	Ion Series: 309.37--585.34--698.42
002.89	0717.59	0.02	40.22-40.29	1147-1149	Ion Series: 310.12--439.19--585.92
002.59	0934.75	0.53	79.67-79.75	2259-2261	Ion Series: 779.61--1055.60--1169.
002.56	0608.61	0.39	61.43-61.50	1743-1745	Ion Series: 544.40--691.54--804.47
002.38	0751.56	0.65	68.80-68.88	1951-1953	Ion Series: 416.42--544.88--707.75
002.37	0571.50	0.50	67.08-67.15	1903-1905	Ion Series: 463.28--610.34--723.38
002.32	1110.49	0.46	126.30-126.39	3531-3533	Ion Series: 1038.03--1201.36--133

FIG. 21